Using Artificial Intelligence Graph Neural Networks To Repurpose Pre-existing Drugs and Analyze Drug Relationships: Year 2

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As burgeoning crises have exposed failures of the drug discovery cycle - an inability to quickly and effectively develop new drugs - artificial intelligence-based drug repositioning models are emerging as an effective, less capital-intensive way to repurpose pre-existing drugs to treat new conditions. Two computational models were developed using data from DrugBank and deepSNAP libraries. The first model takes in user input regarding the effects of a condition and successfully provides suitable drug candidates, developing novel relationships by analyzing which drugs treat similar effects to the condition being researched. The second model consists of two artificial intelligence graph neural networks (GNNs). The GNNs consist of tens of thousands of nodes, representing drugs, and edges, representing relationships between drugs. This model can penalize and train itself to become more accurate. One GNN can successfully predict drug compatibility with accuracies up to 84% and the other can successfully predict FDA approval of drugs with accuracies up to 81%. Both models were additionally supplemented with an extra 10-15 thousand data points and other drug features such as drug-protein relationships and chemical structures to increase both accuracy and functionality. In addition to this, an application and dynamic user interface was created which packages both models into something that can be directly used by physicians and pharmaceutical companies. With the addition of the user interface and GNN to predict FDA approval, new opportunities for applications have been created including drug personalization, helping pharmaceutical companies and physicians with the user interface, and helping with pandemics and crisis response.

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